What is claimed is:

1. A molecule or molecular complex comprising at least a portion of an *S. aureus* FemA or *S. aureus* FemA-like substrate binding surface, wherein the substrate binding surface comprises amino acids listed in Table 2, the substrate binding surface being defined by a set of points having a root mean square deviation of less than about 1.5 Å from points representing the backbone atoms of said amino acids as represented by the structure coordinates listed in Table 1.

2. A molecule or molecular complex comprising at least a portion of an *S. aureus* FemA or *S. aureus* FemA-like binding site, wherein the binding site comprises the amino acids listed in Table 3, the binding site being defined by a set of points having a root mean square deviation of less than about 1.5 Å from points representing the backbone atoms of said amino acids as represented by the structure coordinates listed in Table 1.

3. The molecule or molecular complex of claim 2, wherein the binding site is a binding site for coenzyme A.

4. A molecule or molecular complex comprising at least a portion of an *S. aureus* FemA or *S. aureus* FemA-like binding site, wherein the binding site comprises the amino acids listed in Table 4, the binding site being defined by a set of points having a root mean square deviation of less than about 1.5 Å from points representing the backbone atoms of said amino acids as represented by the structure coordinates listed in Table 1.

5. The molecule or molecular complex of claim 4, wherein the binding site is a binding site for coenzyme A.

6. A molecule or molecular complex that is structurally homologous to an *S. aureus* FemA molecule or molecular complex, wherein the *S. aureus* FemA molecule or molecular complex is represented by at least a portion of the structure coordinates listed in Table 1.

7. A scalable three dimensional configuration of points, at least a portion of said points being derived from structure coordinates listed in Table 1 of at least a portion of an *S. aureus* FemA molecule or molecular complex comprising at least one of a FemA or FemA-like binding site or substrate binding surface.

8. The scalable three dimensional configuration of points of claim 7, wherein substantially all of said points are derived from structure coordinates listed in Table 1 of an *S. aureus* FemA molecule or molecular complex.

9. The scalable three dimensional configuration of points of claim 7 wherein at least a portion of the points derived from the *S. aureus* FemA structure coordinates are derived from structure coordinates representing the locations of at least the backbone atoms of amino acids defining an *S. aureus* FemA substrate binding surface, the substrate binding surface comprising the amino acids listed in Table 2.

10. The scalable three dimensional configuration of points of claim 7 wherein at least a portion of the points derived from the *S. aureus* FemA structure coordinates are derived from structure coordinates representing the locations of at least the backbone atoms of amino acids defining an *S. aureus* FemA binding site, the binding site comprising the amino acids listed in Table 3.

11. The scalable three dimensional configuration of points of claim 10, wherein the binding site is a binding site for coenzyme A.

12. The scalable three dimensional configuration of points of claim 7 wherein at least a portion of the points derived from the *S. aureus* FemA structure coordinates are derived from structure coordinates representing the locations of at least the backbone atoms of amino acids defining an *S. aureus* FemA binding site, the binding site comprising the amino acids listed in Table 4.

13. The scalable three dimensional configuration of points of claim 12, wherein the binding site is a binding site for coenzyme A.

14. The scalable three dimensional configuration of points of claim 7 displayed as a holographic image, a stereodiagram, a model or a computer-displayed image.

15. A scalable three dimensional configuration of points, at least a portion of the points derived from structure coordinates of at least a portion of a molecule or a molecular complex that is structurally homologous to an *S. aureus* FemA molecule or molecular complex and comprises at least one of an *S. aureus* FemA or *S. aureus* FemA-like binding site or substrate binding surface.

16. The scalable three-dimensional configuration of points of claim 15 displayed as a holographic image, a stereodiagram, a model or a computer-displayed image.

17. A machine-readable data storage medium comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, displays a graphical three-dimensional representation of at least one molecule or molecular complex selected from the group consisting of:

(i) a molecule or molecular complex comprising at least a portion of an *S. aureus* FemA or *S. aureus* FemA-like substrate binding surface comprising the amino acids listed in Table 2, the substrate binding surface being defined by a set of

points having a root mean square deviation of less than about 1.5 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1;

(ii) a molecule or molecular complex comprising at least a portion of an *S. aureus* FemA or *S. aureus* FemA-like binding site comprising the amino acids listed in Table 3, the binding site being defined by a set of points having a root mean square deviation of less than about 1.5 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1;

(iii) a molecule or molecular complex comprising at least a portion of an *S. aureus* FemA or *S. aureus* FemA-like binding site comprising the amino acids listed in Table 4, the binding site being defined by a set of points having a root mean square deviation of less than about 1.5 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1; and

(iv) a molecule or molecular complex that is structurally homologous to an *S. aureus* FemA molecule or molecular complex, wherein the *S. aureus* FemA molecule or molecular complex is represented by at least a portion of the structure coordinates listed in Table 1.

18. A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of machine readable data, using a machine programmed with instructions for using said first set of data and said second set of data, determines at least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein said first set of data comprises a Fourier transform of at least a portion of the structure coordinates for *S. aureus* FemA listed in Table 1; and said second set of data comprises an x-ray diffraction pattern of a molecule or molecular complex of unknown structure.

19. A method for obtaining structural information about a molecule or a molecular complex of unknown structure comprising:

crystallizing the molecule or molecular complex;

generating an x-ray diffraction pattern from the crystallized molecule or molecular complex; and

applying at least a portion of the structure coordinates set forth in Table 1 to the x-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

20. A method for homology modeling an *S. aureus* FemA homolog comprising:

aligning the amino acid sequence of an *S. aureus* FemA homolog with an amino acid sequence of *S. aureus* FemA (SEQ ID NO:1) and incorporating the sequence of the *S. aureus* FemA homolog into a model of *S. aureus* FemA formed from structure coordinates set forth in Table 1 to yield a preliminary model of the *S. aureus* FemA homolog;

subjecting the preliminary model to energy minimization to yield an energy minimized model; and

remodeling regions of the energy minimized model where stereochemistry restraints are violated to yield a final model of the *S. aureus* FemA homolog.

21. A computer-assisted method for identifying a potential modifier of *S. aureus* FemA activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* FemA or *S. aureus* FemA-like substrate binding surface, the substrate binding surface comprising the amino acids listed in Table 2;

supplying the computer modeling application with a set of structure coordinates of a chemical entity; and

determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential modification of *S. aureus* FemA activity.

22. The method of claim 21, wherein the substrate binding surface comprises the amino acids listed in Table 2, the substrate binding surface being defined by a set of points having a root mean square deviation of less than about 1.5 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

23. A computer-assisted method for identifying a potential modifier of *S. aureus* FemA activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* FemA or *S. aureus* FemA-like binding site, the binding site comprising the amino acids listed in Table 3;

supplying the computer modeling application with a set of structure coordinates of a chemical entity; and

determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential modification of *S. aureus* FemA activity.

24. The method of claim 23, wherein the binding site comprises the amino acids listed in Table 3, the binding site being defined by a set of points having a root mean square deviation of less than about 1.5 Å from points representing the

backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

25. A computer-assisted method for identifying a potential modifier of *S. aureus* FemA activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* FemA or *S. aureus* FemA-like binding site, the binding site comprising the amino acids listed in Table 4;

supplying the computer modeling application with a set of structure coordinates of a chemical entity; and

determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential modification of *S. aureus* FemA activity.

26. The method of claim 25, wherein the binding site comprises the amino acids listed in Table 4, the binding site being defined by a set of points having a root mean square deviation of less than about 1.5 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

27. The method of claim 21, 23, or 25, wherein determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex comprises performing a fitting operation between the chemical entity and a binding site or substrate binding surface of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between, or the interference with, the chemical entity and the binding site.

28. The method of claim 21, 23, or 25 further comprising screening a library of chemical entities.

29. A computer-assisted method for designing a potential modifier of *S. aureus* FemA activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* FemA or *S. aureus* FemA-like substrate binding surface, the substrate binding surface comprising the amino acids listed in Table 2;

supplying the computer modeling application with a set of structure coordinates for a chemical entity;

evaluating the potential binding or interfering interactions between the chemical entity and the substrate binding surface of the molecule or molecular complex;

structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and

determining whether the modified chemical entity is expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential modification of *S. aureus* FemA activity.

30. The method of claim 29, wherein the substrate binding surface comprises the amino acids listed in Table 2, the substrate binding surface being defined by a set of points having a root mean square deviation of less than about 1.5 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

31. A computer-assisted method for designing a potential modifier of *S. aureus* FemA activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* FemA or *S. aureus* FemA-like binding site, the binding site comprising the amino acids listed in Table 3;

supplying the computer modeling application with a set of structure coordinates for a chemical entity;

evaluating the potential binding or interfering interactions between the chemical entity and the binding site of the molecule or molecular complex;

structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and

determining whether the modified chemical entity is expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential modification of *S. aureus* FemA activity.

32. The method of claim 31, wherein the binding site comprises the amino acids listed in Table 3, the binding site being defined by a set of points having a root mean square deviation of less than about 1.5 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

33. A computer-assisted method for designing a potential modifier of *S. aureus* FemA activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* FemA or *S. aureus* FemA-like binding site, the binding site comprising the amino acids listed in Table 4;

supplying the computer modeling application with a set of structure coordinates for a chemical entity;

evaluating the potential binding or interfering interactions between the chemical entity and the binding site of the molecule or molecular complex;

structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and

determining whether the modified chemical entity is expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential modification of *S. aureus* FemA activity.

34. The method of claim 33, wherein the binding site comprises the amino acids listed in Table 4, the binding site being defined by a set of points having a root mean square deviation of less than about 1.5 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

35. The method of claim 29, 31, or 33, wherein determining whether the modified chemical entity is expected to bind to or interfere with the molecule or molecular complex comprises performing a fitting operation between the chemical entity and a binding site or substrate binding surface of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between or interference with the chemical entity and the binding site or substrate binding surface.

36. The method of claim 29, 31, or 33, wherein the set of structure coordinates for the chemical entity is obtained from a chemical fragment library

37. A computer-assisted method for designing a potential modifier of *S. aureus* FemA activity *de novo* comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* FemA substrate binding surface, wherein the substrate binding surface comprises the amino acids listed in Table 2;

computationally building a chemical entity represented by set of structure coordinates; and

determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential modification of *S. aureus* FemA activity.

38. The method of claim 37, wherein the substrate binding surface comprises the amino acids listed in Table 2, the substrate binding surface being defined by a set of points having a root mean square deviation of less than about 1.5 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

39. A computer-assisted method for designing a potential modifier of *S. aureus* FemA activity *de novo* comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* FemA or *S. aureus* FemA-like binding site, wherein the binding site comprises the amino acids listed in Table 3;

computationally building a chemical entity represented by set of structure coordinates; and

determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential modification of *S. aureus* FemA activity.

40. The method of claim 39, wherein the binding site comprises the amino acids listed in Table 3, the binding site being defined by a set of points having a root mean square deviation of less than about 1.5 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

41. A computer-assisted method for designing a potential modifier of *S. aureus* FemA activity *de novo* comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* FemA or *S. aureus* FemA-like binding site, wherein the binding site comprises the amino acids listed in Table 4;

computationally building a chemical entity represented by set of structure coordinates; and

determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential modification of *S. aureus* FemA activity.

42. The method of claim 41, wherein the binding site comprises the amino acids listed in Table 4, the binding site being defined by a set of points having a root mean square deviation of less than about 1.5 Å from points representing the

backbone atoms of said amino acids as represented by structure coordinates listed in Table 1.

43. The method of claim 37, 39, or 41, wherein determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex comprises performing a fitting operation between the chemical entity and a binding site of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between or interference with the chemical entity and the binding site.

44. The method of any of claims 21, 23, 25, 29, 31, 33, 37, 39, or 41 further comprising supplying or synthesizing the chemical entity, then assaying the chemical entity to determine whether it modifies *S. aureus* FemA activity.

45. A method for making a potential modifier of *S. aureus* FemA activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield a potential modifier of *S. aureus* FemA activity, the chemical entity having been identified during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of a *S. aureus* FemA or *S. aureus* FemA-like binding site or substrate binding surface; supplying the computer modeling application with a set of structure coordinates of a chemical entity; and determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex at a binding site or substrate binding surface, wherein binding to or interfering with the molecule or molecular complex is indicative of potential modification of *S. aureus* FemA activity.

46. A method for making a potential modifier of *S. aureus* FemA activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield a potential modifier of *S. aureus* FemA activity, the chemical entity having been designed during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of a *S. aureus* FemA or *S. aureus* FemA-like binding site or substrate binding surface; supplying the computer modeling application with a set of structure coordinates for a chemical entity; evaluating the potential binding interactions between the chemical entity and a binding site or substrate binding surface of the molecule or molecular complex; structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex at the binding site, wherein binding to or interfering with the molecule or molecular complex is indicative of potential modification of *S. aureus* FemA activity.

47. A method for making a potential modifier of *S. aureus* FemA activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield a potential modifier of *S. aureus* FemA activity, the chemical entity having been designed during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of a *S. aureus* FemA or *S. aureus* FemA-like binding site or substrate binding surface; computationally building a chemical entity represented by set of structure coordinates; and determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex at a binding site or substrate binding surface, wherein binding to or interfering with the molecule or molecular complex is indicative of potential modification of *S. aureus* FemA activity.

48. A potential modifier of *S. aureus* FemA activity identified, designed or made according to the method of any of the claims 21, 23, 25, 29, 31, 33, 37, 39, 41, 45, 46, or 47.

49. A composition comprising a potential modifier of *S. aureus* FemA activity identified, designed or made according to the method of any of claims 21, 23, 25, 29, 31, 33, 37, 39, 41, 45, 46, or 47.

50. A pharmaceutical composition comprising a potential modifier of *S. aureus* FemA activity identified or designed according to the method of any of claims 21, 23, 25, 29, 31, 33, 37, 39, 41, 45, 46, or 47 or a salt thereof, and pharmaceutically acceptable carrier.

51. A method for crystallizing an *S. aureus* FemA molecule or molecular complex comprising:

preparing purified *S. aureus* FemA at a concentration of about 1 mg/ml to about 50 mg/ml; and

crystallizing *S. aureus* FemA from a solution comprising about 1 wt. % to about 50 wt. % PEG, 0 wt. % to about 50 wt. % glycerol, 0 M to about 1 M NaCl, 0 wt. % to about 40 wt. % DMSO, about 100 mM to about 1 M $Ca(OAc)_2$ and/or $MgCl_2$, and buffered to a pH of about 7 to about 10.

52. A crystal of *S. aureus* FemA.

53. The crystal of claim 52 having the orthorhombic space group symmetry $P2_12_12_1$.

54. The crystal of claim 52 comprising a unit cell having dimensions a, b, and c; wherein a is about 40 Å to about 70 Å, b is about 75 Å to about 105 Å, and c is about 95 Å to about 125 Å; and $\alpha = \beta = \gamma = 90°$.

55. The crystal of claim 52 comprising atoms arranged in a spatial relationship represented by the structure coordinates listed in Table 1.

56. The crystal of claim 52 including amino acids having the sequence SEQ ID NO:1.

57. The crystal of claim 52 having amino acid sequence SEQ ID NO:1, with the proviso that at least one methionine is replaced with selenomethionine.